Description

This Raman database contains spectra of pure organic chemical compounds, including simple aliphatic, aromatic, alicyclic, and heterocyclic compounds, as well as numerous complex materials.

The database can be used a reference in the identification, verification, and classification of unknown compounds. It is also useful in the establishment of complex chemical classes of undocumented commercial compounds with similar structures.

Additional Information

The following information is supplied for each record when available: name, synonyms, CAS Registry Number, catalog number, lot number, source of spectrum, source of sample, instrument name, technique, Raman corrections, Raman laser source, Raman laser wavelength, melting point, boiling point, flash point, density, sample type, physical state, purity, storage requirements, molecular weight, and molecular formula. Molecular structures are also available with the database.

Technique

Every effort is made to maintain the highest standard of accuracy for spectra placed in the Sadtler collections. Each compound was prepared under standard conditions at Bio-Rad Laboratories, Informatics Division Laboratories.

All spectra were measured on a Bruker MultiRAM Stand Alone FT-Raman spectrometer. The FT-Raman instrument employs a 1W Nd:YAG air-cooled laser to deliver an excitation wavelength of 1064 nm. The use of this excitation is particularly useful for the analysis of samples that fluoresce when excited with other high energy visible excitation lines. The detector is a liquid nitrogen cooled germanium detector with a spectral range of 3600 to 50 cm⁻¹ (stokes). The detector offers ultra-low signal detection with minimal noise. The spectra are displayed with a spectral range of 3400 to 150 cm⁻¹ (stokes).

Samples were checked to ensure that non-linearity was avoided to maximize reproducibility and provide for the best subtraction of reference spectra. Any spectra with evidence of decomposition, impurities, or reaction with sampling apparatus were rejected.

Each spectrum was then reviewed independently before inclusion in the database. These quality control procedures provide the best sample purity and structural formula confirmation available for the broad range of compounds in the collection.

This collection has been subject to the Sadtler Data Review Protocol™ to provide you with the highest standard in spectral data today. These rigorous qualifying procedures start at data acquisition and continue throughout the database development process.